



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:37 PM UTC

PDB ID : 4CAC / pdb_00004cac
Title : REFINED STRUCTURE OF HUMAN CARBONIC ANHYDRASE II AT 2.0
ANGSTROMS RESOLUTION
Authors : Lindahl, M.; Habash, D.; Harrop, S.; Helliwell, D.R.; Liljas, A.
Deposited on : 1991-09-05
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

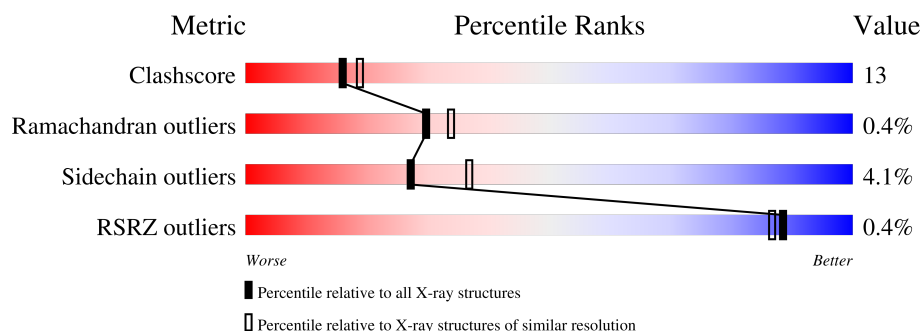
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	259	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2200 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CARBONIC ANHYDRASE FORM C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2039	1309	350	378	2			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

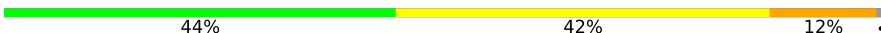
- Molecule 3 is water.

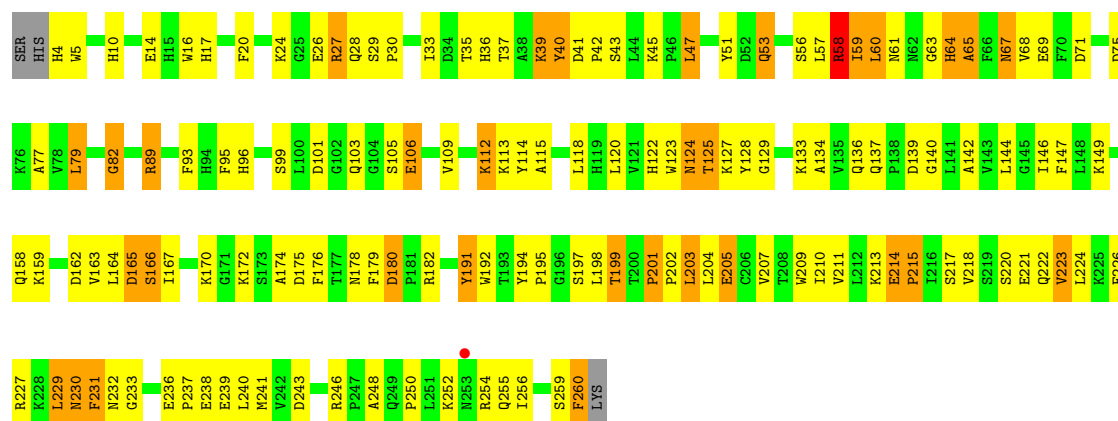
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total	O	0	0
			160	160		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CARBONIC ANHYDRASE FORM C

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.70Å 41.70Å 73.00Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20 70.64 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20) 59.4 (70.64-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.99 (at 2.20Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.187 , (Not available) 0.169 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2200	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5414e-03.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.03	54/2099 (2.6%)	2.28	96/2848 (3.4%)

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	GLY	C-O	7.75	1.34	1.23
1	A	17	HIS	C-N	-7.61	1.24	1.33
1	A	158	GLN	C-O	7.49	1.32	1.24
1	A	218	VAL	C-N	-6.97	1.23	1.33
1	A	254	ARG	C-N	-6.89	1.24	1.33
1	A	248	ALA	C-O	6.64	1.31	1.23
1	A	146	ILE	CA-C	6.62	1.60	1.52
1	A	205	GLU	CA-CB	6.59	1.61	1.52
1	A	16	TRP	NE1-CE2	6.58	1.44	1.37
1	A	4	HIS	C-N	-6.32	1.25	1.33
1	A	238	GLU	N-CA	-6.31	1.38	1.46
1	A	180	ASP	N-CA	6.27	1.55	1.46
1	A	175	ASP	C-O	6.13	1.31	1.23
1	A	133	LYS	N-CA	6.06	1.53	1.46
1	A	93	PHE	C-N	-5.99	1.25	1.33
1	A	254	ARG	NE-CZ	-5.98	1.26	1.33
1	A	233	GLY	N-CA	5.92	1.52	1.45
1	A	240	LEU	CA-C	-5.90	1.45	1.52
1	A	36	HIS	C-O	5.90	1.31	1.24
1	A	139	ASP	CA-C	5.86	1.60	1.53
1	A	109	VAL	N-CA	5.78	1.53	1.46
1	A	256	ILE	C-O	5.73	1.30	1.24
1	A	218	VAL	CA-C	5.73	1.59	1.52
1	A	115	ALA	C-O	5.71	1.31	1.24
1	A	129	GLY	N-CA	-5.65	1.37	1.45
1	A	56	SER	N-CA	5.65	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	TRP	C-O	5.62	1.30	1.24
1	A	197	SER	N-CA	5.60	1.54	1.46
1	A	201	PRO	C-O	5.60	1.30	1.24
1	A	113	LYS	N-CA	-5.55	1.39	1.46
1	A	136	GLN	CA-C	-5.50	1.45	1.52
1	A	227	ARG	NE-CZ	5.50	1.39	1.33
1	A	64	HIS	N-CA	5.49	1.52	1.46
1	A	166	SER	CA-CB	5.47	1.62	1.53
1	A	250	PRO	CA-C	-5.45	1.46	1.52
1	A	236	GLU	C-O	5.38	1.29	1.24
1	A	260	PHE	C-O	5.32	1.34	1.23
1	A	146	ILE	C-O	5.29	1.29	1.24
1	A	5	TRP	N-CA	5.26	1.52	1.46
1	A	59	ILE	N-CA	5.25	1.52	1.46
1	A	256	ILE	CA-C	-5.17	1.46	1.52
1	A	259	SER	C-N	-5.17	1.26	1.33
1	A	158	GLN	C-N	-5.17	1.27	1.33
1	A	125	THR	CA-CB	5.16	1.62	1.53
1	A	40	TYR	C-O	5.15	1.30	1.23
1	A	105	SER	N-CA	5.12	1.52	1.45
1	A	112	LYS	CA-C	5.12	1.59	1.52
1	A	170	LYS	N-CA	5.09	1.52	1.46
1	A	33	ILE	N-CA	5.07	1.52	1.46
1	A	47	LEU	CA-CB	-5.07	1.45	1.53
1	A	61	ASN	C-O	5.07	1.30	1.24
1	A	192	TRP	CA-C	5.05	1.58	1.52
1	A	77	ALA	C-O	5.05	1.29	1.24
1	A	82	GLY	CA-C	5.05	1.59	1.51

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ASP	CA-CB-CG	12.86	125.46	112.60
1	A	230	ASN	CA-CB-CG	12.29	124.89	112.60
1	A	125	THR	CA-C-O	11.31	133.75	119.05
1	A	166	SER	N-CA-C	11.19	124.80	111.82
1	A	58	ARG	NE-CZ-NH1	9.86	131.36	121.50
1	A	231	PHE	CA-CB-CG	9.84	123.64	113.80
1	A	4	HIS	CA-CB-CG	9.27	123.07	113.80
1	A	14	GLU	CB-CG-CD	9.18	128.21	112.60
1	A	226	PHE	CA-CB-CG	9.16	122.96	113.80
1	A	77	ALA	CA-C-O	-9.15	110.79	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ASP	CA-CB-CG	8.89	121.49	112.60
1	A	68	VAL	N-CA-C	-8.55	95.50	107.99
1	A	67	ASN	CA-CB-CG	8.44	121.03	112.60
1	A	53	GLN	CB-CG-CD	-7.94	99.10	112.60
1	A	58	ARG	NE-CZ-NH2	-7.92	112.08	119.20
1	A	218	VAL	CA-C-O	-7.90	113.81	121.63
1	A	201	PRO	CB-CA-C	7.58	120.17	110.92
1	A	95	PHE	CA-CB-CG	7.47	121.27	113.80
1	A	93	PHE	CA-CB-CG	7.39	121.19	113.80
1	A	68	VAL	CA-C-O	-7.25	112.68	120.59
1	A	162	ASP	N-CA-C	7.22	120.01	111.71
1	A	203	LEU	N-CA-CB	-7.07	101.40	112.08
1	A	236	GLU	O-C-N	6.94	127.44	121.20
1	A	254	ARG	N-CA-C	-6.86	101.28	110.55
1	A	194	TYR	O-C-N	6.84	127.94	121.71
1	A	53	GLN	CG-CD-NE2	-6.80	106.20	116.40
1	A	199	THR	O-C-N	6.74	130.77	122.34
1	A	53	GLN	CA-CB-CG	-6.69	100.71	114.10
1	A	207	VAL	N-CA-C	6.63	118.14	108.53
1	A	192	TRP	N-CA-CB	6.60	122.32	110.83
1	A	191	TYR	N-CA-C	6.42	118.71	109.14
1	A	20	PHE	O-C-N	6.39	127.12	121.37
1	A	10	HIS	CA-CB-CG	-6.39	107.41	113.80
1	A	214	GLU	CA-C-N	6.34	126.86	120.14
1	A	214	GLU	C-N-CA	6.34	126.86	120.14
1	A	103	GLN	CA-C-O	-6.29	114.50	121.23
1	A	158	GLN	CA-C-N	6.22	128.91	120.38
1	A	158	GLN	C-N-CA	6.22	128.91	120.38
1	A	223	VAL	O-C-N	6.21	127.89	121.87
1	A	162	ASP	CA-CB-CG	-6.17	106.43	112.60
1	A	175	ASP	N-CA-C	-6.17	101.28	110.23
1	A	237	PRO	CA-C-N	6.15	129.56	120.95
1	A	237	PRO	C-N-CA	6.15	129.56	120.95
1	A	246	ARG	CB-CA-C	-6.10	100.27	108.87
1	A	26	GLU	CB-CA-C	-6.06	97.89	109.95
1	A	222	GLN	CA-C-N	6.03	128.72	120.46
1	A	222	GLN	C-N-CA	6.03	128.72	120.46
1	A	175	ASP	O-C-N	5.98	130.22	122.87
1	A	27	ARG	CD-NE-CZ	-5.95	116.07	124.40
1	A	233	GLY	N-CA-C	-5.92	103.53	112.89
1	A	180	ASP	CB-CA-C	5.91	116.59	109.85
1	A	158	GLN	CA-C-O	-5.90	114.26	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	SER	CB-CA-C	-5.84	99.46	110.67
1	A	61	ASN	CA-C-O	-5.79	114.38	120.58
1	A	236	GLU	CB-CG-CD	5.75	122.37	112.60
1	A	215	PRO	N-CA-CB	5.74	108.72	103.15
1	A	89	ARG	CD-NE-CZ	-5.71	116.40	124.40
1	A	58	ARG	CD-NE-CZ	5.71	132.40	124.40
1	A	36	HIS	CA-CB-CG	-5.66	108.14	113.80
1	A	59	ILE	CB-CA-C	5.65	119.20	110.50
1	A	236	GLU	CA-C-O	-5.64	114.61	120.87
1	A	26	GLU	N-CA-C	5.55	119.90	113.18
1	A	96	HIS	CA-CB-CG	-5.54	108.27	113.80
1	A	165	ASP	CA-C-N	5.51	128.68	120.31
1	A	165	ASP	C-N-CA	5.51	128.68	120.31
1	A	178	ASN	CA-C-O	-5.50	114.74	121.28
1	A	211	VAL	O-C-N	5.46	129.49	123.10
1	A	175	ASP	CA-C-O	-5.46	115.19	121.19
1	A	243	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	37	THR	CA-CB-CG2	5.43	119.73	110.50
1	A	120	LEU	CA-C-O	-5.42	114.90	120.54
1	A	68	VAL	N-CA-CB	5.42	117.55	111.21
1	A	28	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	A	35	THR	N-CA-C	5.41	118.98	112.38
1	A	47	LEU	N-CA-C	-5.40	102.89	110.50
1	A	231	PHE	N-CA-CB	5.35	118.18	110.20
1	A	176	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	106	GLU	CG-CD-OE1	5.31	130.61	118.40
1	A	124	ASN	OD1-CG-ND2	5.28	127.88	122.60
1	A	223	VAL	CA-C-O	-5.26	115.48	120.95
1	A	67	ASN	CA-C-N	-5.25	116.18	122.90
1	A	67	ASN	C-N-CA	-5.25	116.18	122.90
1	A	260	PHE	CA-C-O	-5.23	111.90	120.80
1	A	99	SER	N-CA-C	-5.21	106.77	113.23
1	A	142	ALA	CA-C-O	-5.19	114.74	120.24
1	A	118	LEU	O-C-N	5.18	129.25	123.19
1	A	39	LYS	N-CA-CB	-5.16	102.47	110.57
1	A	197	SER	N-CA-CB	-5.14	101.61	110.87
1	A	198	LEU	N-CA-C	-5.14	103.25	110.50
1	A	147	PHE	CA-C-O	-5.13	115.56	121.47
1	A	63	GLY	CA-C-O	-5.08	113.56	119.10
1	A	103	GLN	N-CA-CB	-5.08	103.69	111.56
1	A	139	ASP	O-C-N	5.07	129.00	122.20
1	A	147	PHE	CA-CB-CG	5.05	118.85	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	231	PHE	N-CA-C	-5.03	105.51	111.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2039	0	1988	53	0
2	A	1	0	0	0	0
3	A	160	0	0	6	0
All	All	2200	0	1988	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.57	1.01
1:A:125:THR:C	1:A:127:LYS:N	2.18	1.01
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.01	0.94
1:A:125:THR:C	1:A:127:LYS:CA	2.54	0.81
1:A:163:VAL:O	1:A:166:SER:HB2	1.83	0.77
1:A:137:GLN:OE1	3:A:394:HOH:O	2.06	0.71
1:A:89:ARG:HG3	1:A:125:THR:CG2	2.21	0.71
1:A:231:PHE:CE1	1:A:241:MET:HG3	2.34	0.63
1:A:75:ASP:OD1	1:A:89:ARG:NE	2.23	0.61
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.36	0.60
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.85	0.59
1:A:112:LYS:HE3	1:A:114:TYR:CZ	2.40	0.57
1:A:134:ALA:O	1:A:140:GLY:HA3	2.05	0.56
1:A:27:ARG:HD3	3:A:293:HOH:O	2.05	0.56
1:A:82:GLY:HA2	1:A:191:TYR:OH	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:THR:C	1:A:127:LYS:HA	2.32	0.55
1:A:195:PRO:HG3	3:A:282:HOH:O	2.05	0.55
1:A:164:LEU:HB3	1:A:229:LEU:HD11	1.88	0.55
1:A:40:TYR:HE2	1:A:42:PRO:HB3	1.70	0.55
1:A:89:ARG:HG3	1:A:125:THR:HG22	1.88	0.54
1:A:159:LYS:CE	3:A:420:HOH:O	2.56	0.53
1:A:144:LEU:HD23	1:A:210:ILE:HB	1.90	0.52
1:A:30:PRO:HG3	1:A:106:GLU:HB3	1.91	0.51
1:A:149:LYS:O	1:A:217:SER:HA	2.10	0.51
1:A:40:TYR:CE2	1:A:42:PRO:HB3	2.47	0.49
1:A:41:ASP:C	1:A:41:ASP:OD1	2.54	0.49
1:A:167:ILE:O	1:A:167:ILE:HG13	2.13	0.47
1:A:231:PHE:HD2	1:A:239:GLU:HG2	1.79	0.47
1:A:64:HIS:O	1:A:65:ALA:HB2	2.15	0.47
1:A:41:ASP:CG	1:A:43:SER:HG	2.21	0.47
1:A:202:PRO:HG2	1:A:204:LEU:HG	1.97	0.46
1:A:201:PRO:HA	1:A:203:LEU:HG	1.97	0.46
1:A:213:LYS:HD3	1:A:260:PHE:CE1	2.49	0.45
1:A:106:GLU:OE1	1:A:199:THR:OG1	2.28	0.45
1:A:180:ASP:OD2	1:A:182:ARG:NH2	2.48	0.45
1:A:124:ASN:OD1	1:A:127:LYS:N	2.49	0.45
1:A:213:LYS:CD	1:A:260:PHE:CZ	2.88	0.45
1:A:123:TRP:CZ3	1:A:125:THR:HA	2.52	0.44
1:A:165:ASP:HB2	3:A:414:HOH:O	2.17	0.44
1:A:230:ASN:HB3	1:A:232:ASN:OD1	2.17	0.44
1:A:59:ILE:HA	1:A:67:ASN:O	2.18	0.43
1:A:60:LEU:HD12	1:A:172:LYS:O	2.20	0.42
1:A:51:TYR:OH	1:A:122:HIS:NE2	2.45	0.42
1:A:252:LYS:NZ	3:A:361:HOH:O	2.52	0.42
1:A:57:LEU:HD11	1:A:71:ASP:HB2	2.02	0.42
1:A:29:SER:HB3	1:A:30:PRO:HA	2.02	0.41
1:A:47:LEU:HD22	1:A:79:LEU:HD21	2.01	0.41
1:A:220:SER:O	1:A:224:LEU:HG	2.21	0.41
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.87	0.41
1:A:47:LEU:HD11	1:A:210:ILE:HG21	2.02	0.41
1:A:45:LYS:O	1:A:82:GLY:HA2	2.21	0.40
1:A:58:ARG:HB2	1:A:174:ALA:O	2.21	0.40
1:A:223:VAL:O	1:A:223:VAL:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/259 (97%)	244 (97%)	7 (3%)	1 (0%)	30	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/224 (99%)	212 (96%)	9 (4%)	27	37

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	39	LYS
1	A	53	GLN
1	A	58	ARG
1	A	60	LEU
1	A	79	LEU
1	A	221	GLU
1	A	229	LEU
1	A	255	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	74	GLN
1	A	136	GLN
1	A	137	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	125:THR	C	127:LYS	N	2.18

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	256/259 (98%)	-0.20	1 (0%) 88 87	3, 13, 24, 28	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ASN	2.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	262	1/1	0.99	0.02	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.